Study guide: Scientific software engineering with a simple ODE model as example

Hans Petter Langtangen[1,2]

Center for Biomedical Computing, Simula Research Laboratory[1]

Department of Informatics, University of Oslo[2]

Mar 27, 2015

1. From flat program to module with functions

2. Creating user interfaces

3. Performning scientific experiments

Mathematical model problem

$$
\begin{aligned}
u'(t) &= -au(t), \quad t \in (0, T] \\
u(0) &= I
\end{aligned}
$$

Solution by θ-scheme:

$$
u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t} u^n
$$

$\theta = 0$: Forward Euler, $\theta = 1$: Backward Euler, $\theta = 1/2$: Crank-Nicolson (midpoint method)

Many will make a rough, flat program first

```
from numpy import *
from matplotlib.pyplot import *

A = 1
a = 2
T = 4
dt = 0.2
N = int(round(T/dt))
y = zeros(N+1)
t = linspace(0, T, N+1)
theta = 1
y[0] = A
for n in range(0, N):
    y[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*y[n]

y_e = A*exp(-a*t) - y
error = y_e - y
E = sqrt(dt*sum(error**2))
print 'Norm of the error: %.3E' % E
plot(t, y, 'r--o')
t_e = linspace(0, T, 1001)
y_e = A*exp(-a*t_e)
plot(t_e, y_e, 'b-')
legend(['numerical, theta=%g' % theta, 'exact'])
xlabel('t')
ylabel('y')
show()
```

There are major issues with this solution

1. The notation in the program does not correspond exactly to the notation in the mathematical problem: the solution is called `y` and corresponds to u in the mathematical description, the variable `A` corresponds to the mathematical parameter I, `N` in the program is called N_t in the mathematics.
2. There are no comments in the program.

New flat program

```
from numpy import *
from matplotlib.pyplot import *

I = 1
a = 2
T = 4
dt = 0.2
Nt = int(round(T/dt))     # no of time intervals
u = zeros(Nt+1)           # array of u[n] values
t = linspace(0, T, Nt+1)  # time mesh
theta = 1                 # Backward Euler method

u[0] = I                  # assign initial condition
for n in range(0, Nt):    # n=0,1,...,Nt-1
    u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]

# Compute norm of the error
u_e = I*exp(-a*t) - u     # exact u at the mesh points
error = u_e - u
E = sqrt(dt*sum(error**2))
print 'Norm of the error: %.3E' % E

# Compare numerical (u) and exact solution (u_e) in a plot
plot(t, u, 'r--o')               # red dashes w/circles
t_e = linspace(0, T, 1001)       # very fine mesh for u_e
u_e = I*exp(-a*t_e)
plot(t_e, u_e, 'b-')             # blue line for u_e
legend(['numerical, theta=%g' % theta, 'exact'])
```

Such flat programs are ideal for IPython notebooks!

IP[y]: Notebook   Test (autosaved)

File Edit View Insert Cell Kernel Help

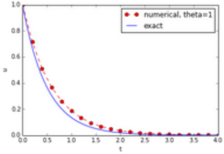
Code   Cell Toolbar: None

In [1]:
```
%matplotlib inline
```

In [4]:
```
from numpy import *
from matplotlib.pyplot import *

I = 1
a = 2
T = 4
dt = 0.2
Nt = int(round(T/dt))     # no of time intervals
u = zeros(Nt+1)           # array of u[n] values
t = linspace(0, T, Nt+1)  # time mesh
theta = 1                 # Backward Euler method
u[0] = I                  # assign initial condition
for n in range(0, Nt):    # n=0,1,...,Nt-1
    u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]

# Compute norm of the error
u_e = I*exp(-a*t) - u     # exact u at the mesh points
error = u_e - u
E = sqrt(dt*sum(error**2))
print 'Norm of the error: %.3E' % E

# Compare numerical (u) and exact solution (u_e) in a plot
plot(t, u, 'r--o')               # red dashes w/circles
t_e = linspace(0, T, 1001)       # very fine mesh for u_e
u_e = I*exp(-a*t_e)
plot(t_e, u_e, 'b-')             # blue line for u_e
legend(['numerical, theta=%g' % theta, 'exact'])
xlabel('t')
ylabel('u')
```

```
Norm of the error: 6.794E-01
```

Out[4]: <matplotlib.text.Text at 0x7fed42052ad0>



In [ ]:

But: Further development of such flat programs require many scattered edits - easy to make mistakes!

The solution formula for u^{n+1} is completely general and should be available as a Python function with all input data as function arguments and all output data returned to the calling code

```
def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    dt = float(dt)               # avoid integer division
    Nt = int(round(T/dt))        # no of time intervals
    T = Nt*dt                    # adjust T to fit time step dt
    u = np.zeros(Nt+1)           # array of u[n] values
    t = np.linspace(0, T, Nt+1)  # time mesh

    u[0] = I                   # assign initial condition
    for n in range(0, Nt):     # n=0,1,...,Nt-1
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

Call:

```
u, t = solver(I=1, a=2, T=4, dt=0.2, theta=0.5)
```

The DRY principle: Don't repeat yourself!

DRY:

When implementing a particular functionality in a computer program, make sure this functionality and its variations are implemented in just one piece of code. That is, if you need to revise the implementation, there should be *one and only one* place to edit. It follows that you should never duplicate code (don't repeat yourself!), and code snippets that are similar should be factored into one piece (function) and parameterized (by function arguments).

Make sure any program file is a valid Python module

- Module requires code to be divided into functions :-)
- Why module? Other programs can import the functions

```
from decay import solver
# Solve a decay problem
u, t = solver(I=1, a=2, T=4, dt=0.2, theta=0.5)
```

or prefix function names by the module name:

```
import decay
# Solve a decay problem
u, t = decay.solver(I=1, a=2, T=4, dt=0.2, theta=0.5)
```

The requirements of a module are so simple

1. The filename without .py must be a valid Python variable name.
2. The main program must be executed (through statements or a function call) in the *test block*.

The *test block* is normally placed at the end of a module file:

```
if __name__ == '__main__':
    # Statements
```

If the file is imported, the if test fails and no main program is run, otherwise, the file works as a program

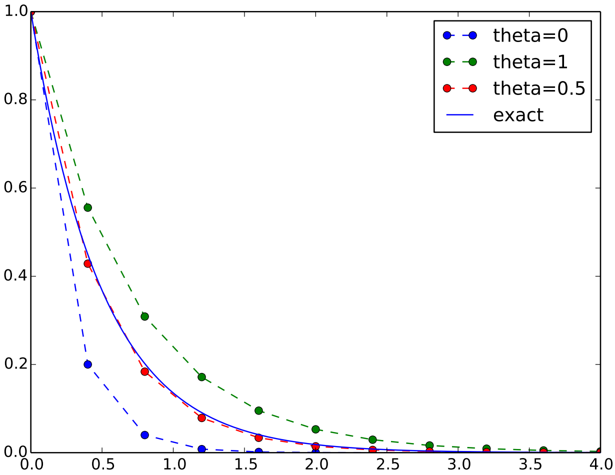
The module file decay.py for our example

```python
from numpy import *
from matplotlib.pyplot import *

def solver(I, a, T, dt, theta):
    ...

def exact_solution(t, I, a):
    return I*exp(-a*t)

def experiment_compare_numerical_and_exact():
    I = 1;  a = 2;  T = 4;  dt = 0.4;  theta = 1
    u, t = solver(I, a, T, dt, theta)

    t_e = linspace(0, T, 1001)        # very fine mesh for u_e
    u_e = exact_solution(t_e, I, a)

    plot(t,   u,   'r--o')            # dashed red line with circles
    plot(t_e, u_e, 'b-')              # blue line for u_e
    legend(['numerical, theta=%g' % theta, 'exact'])
    xlabel('t')
    ylabel('u')
    plotfile = 'tmp'
    savefig(plotfile + '.png');  savefig(plotfile + '.pdf')

    error = exact_solution(t, I, a) - u
    E = sqrt(dt*sum(error**2))
    print 'Error norm:', E
```

The module file decay.py for our example w/prefix

```python
import numpy as np
import matplotlib.pyplot as plt

def solver(I, a, T, dt, theta):
    ...

def exact_solution(t, I, a):
    return I*np.exp(-a*t)

def experiment_compare_numerical_and_exact():
    I = 1;  a = 2;  T = 4;  dt = 0.4;  theta = 1
    u, t = solver(I, a, T, dt, theta)

    t_e = np.linspace(0, T, 1001)        # very fine mesh for u_e
    u_e = exact_solution(t_e, I, a)

    plt.plot(t,   u,   'r--o')       # dashed red line with circles
    plt.plot(t_e, u_e, 'b-')         # blue line for u_e
    plt.legend(['numerical, theta=%g' % theta, 'exact'])
    plt.xlabel('t')
    plt.ylabel('u')
    plotfile = 'tmp'
    plt.savefig(plotfile + '.png');  plt.savefig(plotfile + '.pdf')

    error = exact_solution(t, I, a) - u
    E = np.sqrt(dt*np.sum(error**2))
    print 'Error norm:', E
```

How do we add code for comparing schemes visually?



Think of edits in the flat program that are required to produce this plot (!)

We just add a new function with the tailored plotting

```
def experiment_compare_schemes():
    """Compare theta=0,1,0.5 in the same plot."""
    I = 1;  a = 2;  T = 4;  dt = 0.4
    legends = []
    for theta in [0, 1, 0.5]:
        u, t = solver(I, a, T, dt, theta)
        plt.plot(t, u, '--o')                  # dashed lines with circles
        legends.append('theta=%g' % theta)
    t_e = np.linspace(0, T, 1001)              # very fine mesh for u_e
    u_e = exact_solution(t_e, I, a)
    plt.plot(t_e, u_e, 'b-')                   # blue line for u_e
    legends.append('exact')
    plt.legend(legends, loc='upper right')
    plotfile = 'tmp'
    plt.savefig(plotfile + '.png');  plt.savefig(plotfile + '.pdf')
```

Prefixing imported functions by the module name

MATLAB-style names (`linspace`, `plot`):

```
from numpy import *
from matplotlib.pyplot import *
```

Python community convention is to prefix with module name (`np.linspace`, `plt.plot`):

```
import numpy as np
import matplotlib.pyplot as plt
```

1. From flat program to module with functions

2. Creating user interfaces

3. Performning scientific experiments

Creating user interfaces

- Never edit the program to change input!
- Set input data on the command line or in a graphical user interface
- How is explained next

Accessing command-line arguments

- All command-line arguments are available in `sys.argv`
- `sys.argv[0]` is the program
- `sys.argv[1:]` holds the command-line arguments
- Method 1: fixed sequence of parameters on the command line
- Method 2: `--option value` pairs on the command line (with default values)

```
Terminal> python myprog.py 1.5 2 0.5 0.8 0.4
Terminal> python myprog.py --I 1.5 --a 2 --dt 0.8 0.4
```

Reading a sequence of command-line arguments

Required input:

- I
- a
- T
- name of scheme (FE, BE, CN)
- a list of Δt values

Give these on the command line in correct sequence

```
Terminal> python decay_cml.py 1.5 0.5 4 CN 0.1 0.2 0.05
```

Implementation

```
def define_command_line_options():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument(
        '--I', '--initial_condition', type=float,
        default=1.0, help='initial condition, u(0)',
        metavar='I')
    parser.add_argument(
        '--a', type=float, default=1.0,
        help='coefficient in ODE', metavar='a')
    parser.add_argument(
        '--T', '--stop_time', type=float,
        default=1.0, help='end time of simulation',
        metavar='T')
    parser.add_argument(
        '--scheme', type=str, default='CN',
        help='FE, BE, or CN')
    parser.add_argument(
        '--dt', '--time_step_values', type=float,
        default=[1.0], help='time step values',
        metavar='dt', nargs='+', dest='dt_values')
    return parser
```

Note:

- `sys.argv[i]` is *always a string*

Working with an argument parser

Set option-value pairs on the command line if the default value is not suitable:

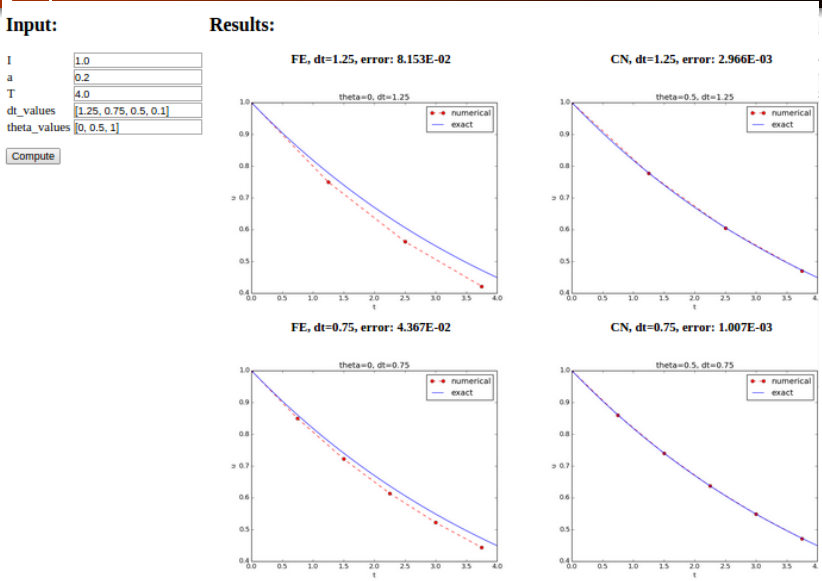
```
Terminal> python decay_argparse.py --I 1.5 --a 2 --dt 0.8 0.4
```

Code:

```
def read_command_line_argparse():
    parser = define_command_line_options()
    args = parser.parse_args()
    scheme2theta = {'BE': 1, 'CN': 0.5, 'FE': 0}
    data = (args.I, args.a, args.T, scheme2theta[args.scheme],
            args.dt_values)
    return data
```

(`metavar` is the symbol used in help output)

A graphical user interface



Normally very much programming required - and much competence on graphical user interfaces.

The Parampool package

- Parampool is a package for handling a large pool of input parameters in simulation programs
- Parampool can automatically create a sophisticated web-based graphical user interface (GUI) to set parameters and view solutions

Remark

The forthcoming material aims at those with particular interest in equipping their programs with a GUI - others can safely skip it.

Making a compute function

- Key concept: a *compute function* that takes all input data as arguments and returning HTML code for viewing the results (e.g., plots and numbers)
- What we have: `decay_plot.py`
- `main` function carries out simulations and plotting for a series of Δt values
- Goal: steer and view these experiments from a web GUI
- What to do:
    - create a compute function
    - call `parampool` functionality

The compute function must return HTML code

```
def main_GUI(I=1.0, a=.2, T=4.0,
             dt_values=[1.25, 0.75, 0.5, 0.1],
             theta_values=[0, 0.5, 1]):
    # Build HTML code for web page. Arrange plots in columns
    # corresponding to the theta values, with dt down the rows
    theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
    html_text = '<table>\n'
    for dt in dt_values:
        html_text += '<tr>\n'
        for theta in theta_values:
            E, html = compute4web(I, a, T, dt, theta)
            html_text += """
<td>
<center><b>%s, dt=%g, error: %.3E</b></center><br>
%s
</td>
""" % (theta2name[theta], dt, E, html)
        html_text += '</tr>\n'
    html_text += '</table>\n'
    return html_text
```

Generating the user interface

Make a file decay_GUI_generate.py:

```
from parampool.generator.flask import generate
from decay import main_GUI
generate(main_GUI,
         filename_controller='decay_GUI_controller.py',
         filename_template='decay_GUI_view.py',
         filename_model='decay_GUI_model.py')
```

Running decay_GUI_generate.py results in

1. decay_GUI_model.py defines HTML widgets to be used to set input data in the web interface,
2. templates/decay_GUI_views.py defines the layout of the web page,
3. decay_GUI_controller.py runs the web application.

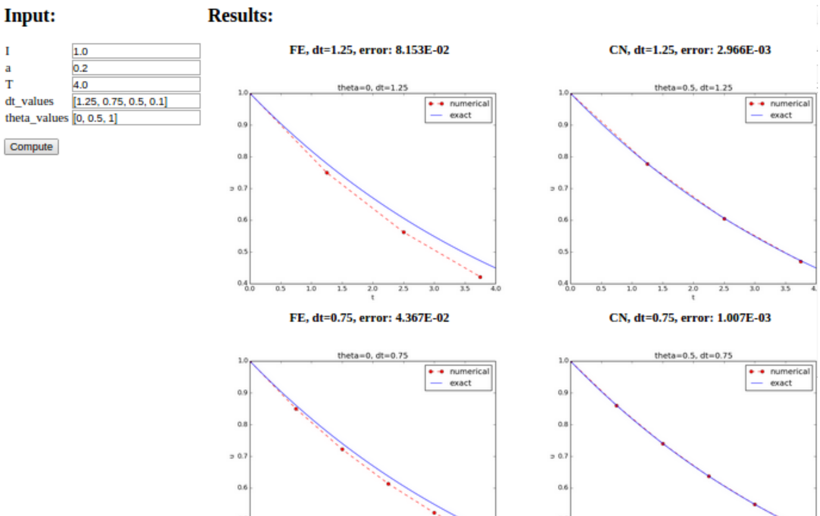
Good news: we only need to run decay_GUI_controller.py and there is no need to look into any of these files!

Running the web application

Start the GUI

```
Terminal> python decay_GUI_controller.py
```

Open a web browser at `127.0.0.1:5000`



More advanced use

- The compute function can have arguments of type float, int, string, list, dict, numpy array, filename (file upload)
- Alternative: specify a hierarchy of input parameters with name, default value, data type, widget type, unit (m, kg, s), validity check
- The generated web GUI can have user accounts with login and storage of results in a database

Doctests

Doc strings can be equipped with interactive Python sessions for demonstrating usage and *automatic testing* of functions.

```
def solver(I, a, T, dt, theta):
    """
    Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt.


    >>> u, t = solver(I=0.8, a=1.2, T=2, dt=0.5, theta=0.5)
    >>> for t_n, u_n in zip(t, u):
    ...     print 't=%.1f, u=%.14f' % (t_n, u_n)
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
    """
    ...
```

Running doctests

Automatic check that the code reproduces the doctest output:

```
Terminal> python -m doctest decay.py
```

Floats are difficult to compare

Limit the number of digits in the output in doctests! Otherwise, round-off errors on a different machine may ruin the test.

Unit testing with nose

- Nose and pytest are a very user-friendly testing frameworks
- Based on *unit testing*
- Identify (small) units of code and test each unit
- Nose automates running all tests
- Good habit: run all tests after (small) edits of a code
- Even better habit: write tests *before* the code (!)
- Remark: unit testing in scientific computing is not yet well established

Basic use of nose and pytest

1. Implement tests in *test functions* with names starting with `test_`.
2. Test functions cannot have arguments.
3. Test functions perform assertions on computed results using `assert` functions from the `nose.tools` module.
4. Test functions can be in the source code files or be collected in separate files `test*.py`.

Example on a test function in the source code

Very simple module mymod (in file mymod.py):

```
def double(n):
    return 2*n
```

Write test function in mymod.py:

```
def double(n):
    return 2*n

def test_double():
    n = 4
    expected = 2*4
    computed = double(n)
    assert expected == computed
```

Running one of

```
Terminal> nosetests -s -v mymod
Terminal> py.test   -s -v mymod
```

makes the framework run all test_*() functions in mymod.py.

Example on test functions in a separate file

Write the test in a separate file, say `test_mymod.py`:

```
import mymod

def test_double():
    n = 4
    expected = 2*4
    computed = double(n)
    assert expected == computed
```

Running one of

```
Terminal> nosetests -s -v
Terminal> py.test   -s -v
```

makes the frameworks run all `test_*()` functions in all files `test*.py` in the current directory and in all subdirectories (pytest) or just those with names `tests` or `*_tests` (nose)

Tip

Start with test functions in the source code file. When the file contains many tests, or when you have many source code files, move tests to separate files.

Test function for solver

Use exact discrete solution of the θ scheme as test:

$$u^n = I\left(\frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}\right)^n$$

```
def exact_discrete_solution(n, I, a, theta, dt):
    """Return exact discrete solution of the numerical schemes."""
    dt = float(dt)  # avoid integer division
    A = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*A**n

def test_exact_discrete_solution():
    """Check that solver reproduces the exact discr. sol."""
    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    Nt = int(8/dt)  # no of steps
    u, t = solver(I=I, a=a, T=Nt*dt, dt=dt, theta=theta)

    # Evaluate exact discrete solution on the mesh
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(Nt+1)])

    # Find largest deviation
    diff = np.abs(u_de - u).max()
    tol = 1E-14
    success = diff < tol
    assert success
```

Can test that potential integer division is avoided too

Warning

If a, Δt, and θ are integers, the formula for u^{n+1} in the solver function may lead to 0 because of unintended integer division.

```
def test_potential_integer_division():
    """Choose variables that can trigger integer division."""
    theta = 1; a = 1; I = 1; dt = 2
    Nt = 4
    u, t = solver(I=I, a=a, T=Nt*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(Nt+1)])
    diff = np.abs(u_de - u).max()
    assert diff < 1E-14
```

1. From flat program to module with functions

2. Creating user interfaces

3. Performning scientific experiments

Performning scientific experiments

Goals:

1. Explore the behavior of a numerical method for an ODE
2. Show how a program can set up, execute, and report scientific investigations
3. Demonstrate how to write a scientific report
4. Demonstrate various technologies for reports: HTML w/MathJax, $\LaTeX$, Sphinx, IPython notebooks, ...

Model problem and numerical solution method

Problem:

$$u'(t) = -au(t), \quad u(0) = I,\ 0 < t \leq T, \tag{1}$$

Solution method (θ-rule):

$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}u^n, \quad u^0 = I\,.$$

Plan for the experiments

For fixed I, a, and T, we run the three schemes for various values of Δt, and present in a report the following results:

1. visual comparison of the numerical and exact solution in a plot for each Δt and $\theta = 0, 1, \frac{1}{2}$,
2. a table and a plot of the norm of the numerical error versus Δt for $\theta = 0, 1, \frac{1}{2}$.

Available software

`model.py`:

```
Terminal> python model.py --I 1.5 --a 0.25 --T 6 --dt 1.25 0.75 0.5
0.0   1.25:    5.998E-01
0.0   0.75:    1.926E-01
0.0   0.50:    1.123E-01
0.0   0.10:    1.558E-02
0.5   1.25:    6.231E-02
0.5   0.75:    1.543E-02
0.5   0.50:    7.237E-03
0.5   0.10:    2.469E-04
1.0   1.25:    1.766E-01
1.0   0.75:    8.579E-02
1.0   0.50:    6.884E-02
1.0   0.10:    1.411E-02
```

+ a set of plot files of numerial vs exact solution

Required new results

- Put plots together in table of plots
- Table of numerical error vs Δt and θ
- Log-log convergence plot of numerical error vs Δt for $\theta = 0, 1, 0.5$

Must write a script `exper1.py` to automate running `model.py` and generating these results

```
Terminal> python exper1.py 0.5 0.25 0.1 0.05
```

(Δt values on the comand line)

Reproducible science is key!

Let your scientific investigations be automated by scripts!

- Excellent documentation
- Trivial to re-run experiments
- Easy to extend investigations

What actions are needed in the script?

1. Run `model.py` program with appropriate input
2. Interpret the output and make table and plot of numerical errors
3. Combine plot files to new figures

Complete script: `exper1.py`

Run a program from a program with subprocess

Command to be run:

```
python model.py --I 1.2 --a 0.2 --T 8 -dt 1.25 0.75 0.5 0.1
```

Constructed in Python:

```
# Given I, a, T, and a list dt_values
cmd = 'python model.py --I %g --a %g --T %g' % (I, a, T)
dt_values_str = ' '.join([str(v) for v in dt_values])
cmd += ' --dt %s' % dt_values_str
```

Run under the operating system:

```
from subprocess import Popen, PIPE, STDOUT
p = Popen(cmd, shell=True, stdout=PIPE, stderr=STDOUT)
output, dummy = p.communicate()

failure = p.returncode
if failure:
    print 'Command failed:', cmd; sys.exit(1)
```

Interpreting the output from an operating system command

The output if the previous command run by subprocess is in a string output:

```
errors = {'dt': dt_values, 1: [], 0: [], 0.5: []}
for line in output.splitlines():
    words = line.split()
    if words[0] in ('0.0', '0.5', '1.0'):  # line with E?
        # typical line: 0.0   1.25:    7.463E+00
        theta = float(words[0])
        E = float(words[2])
        errors[theta].append(E)
```

Combining plot files: PNG and PDF solutions

PNG:

```
Terminal> montage -background white -geometry 100% -tile 2x \
          f1.png f2.png f3.png f4.png f.png
Terminal> convert -trim f.png f.png
Terminal> convert f.png -transparent white f.png
```

PDF:

```
Terminal> pdftk f1.pdf f2.pdf f3.pdf f4.pdf output tmp.pdf
Terminal> pdfnup --nup 2x2 --outfile tmp.pdf tmp.pdf
Terminal> pdfcrop tmp.pdf f.pdf
Terminal> rm -f tmp.pdf
```

Easy to build these commands in Python and execute them with `subprocess` or `os.system`: `os.system(cmd)`

Making a report

- Scientific investigations are best documented in a report!
- A sample report
- How can we write such a report?
- First problem: what format should I write in?
- Plain HTML
- HTML with MathJax
- LaTeX PDF, based on LaTeX source
- Sphinx HTML, based on reStructuredText
- IPython notebook, Markdown, MediaWiki, ...
- DocOnce can generate LaTeX, HTML w/MathJax, Sphinx, IPython notebook, Markdown, MediaWiki, ... (DocOnce source for the examples above)
- Examples on different report formats

Publishing a complete project

- Make folder (directory) tree
- Keep track of all files via a *version control system* (Git!)
- Publish as private or public repository
- Utilize Bitbucket or GitHub
- See the intro to project hosting sites with version control